



Hydrogeological Characterization of Low-permeability Clayey Tills The Role of Sand Lenses

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Hydrogeological Characterization of Low-permeability Clayey Tills - the Role of Sand Lenses



Timo C. Kessler

Hydrogeological Characterization of Low-permeability Clayey Tills – the Role of Sand Lenses

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PhD Thesis
June 2012

DTU Environment
Department of Environmental Engineering
Technical University of Denmark

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– the Role of Sand Lenses**

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The thesis will be available as a pdf-file for downloading from the homepage of the department: www.env.dtu.dk

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PREFACE

The thesis entitled 'Hydrogeological Characterization of Low-permeability Clayey Tills — the Role of Sand Lenses' was submitted to achieve a PhD degree in the field of hydrogeology. The reported study was conducted at the Department of Environmental Engineering at the Technical University of Denmark (DTU ENV) and at the Geological Survey of Denmark and Greenland (GEUS). The PhD project was completed in the period from December 2008 until March 2012 under supervision of Professor Poul L. Bjerg (DTU ENV) and senior researchers Knud Erik Klint and Bertel Nilsson (both GEUS). The work was part of the REMTEC project (Innovative REMediation and assessment TEChnologies for contaminated soil and groundwater) and was funded by the Danish Council for Strategic Research. The content of the thesis is based on three research articles submitted to peer-reviewed journals and one technical note. The thesis includes a summary of the objectives, methods and findings as well as the scientific articles. The articles are referred in the text with the Roman numbers indicated below. In this web-version the articles are not included, but can be obtained from the Library at DTU Environment, Technical University of Denmark, Miljøvej, Building 113, 2800 Kgs. Lyngby, Denmark, library@env.dtu.dk.

- I. Christiansen, C.M., Damgaard, I., Broholm, M.M., Kessler, T.C., Nilsson, B., Klint, K.E.S., Bjerg, P.L. (2010). Comparison of Delivery Methods for Enhanced *In Situ* Remediation in Clay Till. *Ground Water Monitoring & Remediation*, 30 (4), 107-122.
- II. Kessler, T.C., Klint, K.E.S., Nilsson, B., Bjerg, P.L. Characterization of Sand Lenses Embedded in Tills. *Quaternary Science Reviews*, in revision.
- III. Kessler, T.C., Comunian, A., Oriani, F., Renard, P., Nilsson, B., Klint, K.E.S., Bjerg, P.L. Analyzing and Modeling Fine Scale Geological Heterogeneity — an Example of Sand Lenses in Clayey Till. Submitted manuscript.
- IV. Kessler, T.C., Chambon, J.C., Binning, P.J., Nilsson, B., Klint, K.E.S., Bjerg, P.L. (2012). Implications for Risk Assessment of Sand Lenses for Solute Transport in Heterogeneous Clayey Tills. Technical note.

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SUMMARY

The topic of this PhD thesis is an integrated investigation of sand lenses in glacial diamictons. Sand lenses indicate various deposition regimes and glaciotectonic deformation styles and are as such important features in studies of glacial sediments. In a hydrogeological framework, sand lenses further constitute conductive facies within low-permeability tills and are suspected to affect hydraulic conductivity fields and subsurface transport behaviour. The purpose of the study is to characterize sand lenses in terms of occurrence, geometry and connectivity and to assess their importance for contaminant transport in clayey tills.

Sand lenses are considered enigmatic geological features resulting from complex interplay of glacial deposition and deformation. The subglacial hydraulic conditions and the predominant deforming forces are determining the appearance of sand lenses. Despite the abundance and the variability of occurrence, there is only sparse systematic information reported in the literature. As an example there is no consistent nomenclature for the different types of sand and gravel deposits in tills. In this study, the specific geometry of sand lenses was characterized by means of a field observation study and a literature survey. A number of geometric parameters (length, thickness, anisotropy, orientation, etc.) were selected to describe the size and shape of sand lenses. The resulting characteristic measures were used to define a classification scheme and to categorize five types of sand lenses. These are: sand layers, sand sheets, sand bodies, sand pockets and sand stringers. The scheme is a useful tool to include sand lenses in future till investigations and it supports rapid identification of till types.

The spatial distribution of sand lenses is variable because of generally complex architectures of till successions. On the other hand, it is a relevant parameter to describe because mean lengths and spacing determine the connectivity between lenses. Pixel-based mapping of geological cross-sections was performed to facilitate geostatistical analyses of spatial variability. Variogram models yield non-stationary patterns including trending in vertical direction, variable size of lenses and strong geometric anisotropy. Non-stationarity complicates the identification of correlation functions and hampers the simulation of facies distribution. Transition probability-based geostatistics applied abundantly in modeling complex facies architecture were used in this study to simulate the variability of sand lenses in tills. Multiple-point statistics, however, showed enhanced capabilities to repro-

duce characteristic geological structures. Especially strong anisotropy and variable size of sand lenses were best represented in multiple-point realizations. Stochastic models enable the identification of connectivity functions and can be used to simulate heterogeneity at poorly or unsampled locations.

Once the specific structures of sand lenses are reproduced to satisfaction, hydraulic parameters can be assigned to the different geological facies. The average hydraulic conductivity between the sand lenses and the clayey matrix differ by three to four orders of magnitude. The influence of sand lenses on the transport regime thus depends primarily on the connectivity between lenses. Three-dimensional realizations indicate clear channel networks, whereas only limited connectivity was found for the two-dimensional case. This is an important aspect because it emphasizes the need to collect data and to represent this type of heterogeneity in 3D. The physical response of sand lens heterogeneity was evaluated performing solute transport modeling mimicking leaching from a contaminated site in clayey till. It emphasized the need to include geological heterogeneity even if occurring at the finest scale. Compared to average or random conductivity fields, simulated sand lenses with specific hydraulic properties enhance the horizontal spreading of contaminants without a significant increase of the equivalent permeability in the till.

Overall, sand lenses occur in all types of glacial sediments and with a broad range of shapes and hydraulic properties. Geometric characterization enabled classification of the most common types. Geostatistical analyses suggested that sand lenses in tills create connected channel networks in 3D. Consequently, sand lens heterogeneity is an important aspect when modeling transport processes of contaminants or performing risk assessment in clayey till settings. In either case it is recommended to consider and to include detailed representations of heterogeneity and sand lenses.

DANSK RESUMÉ

Denne afhandling omhandler en integreret undersøgelse af sandlinser i glaciale aflejringer. Sandlinser udgør et væsentligt element i studiet af glaciale sedimenter, da de afspejler forskellige aflejningsforhold og glacialtektoniske deformationstyper. Sandlinser findes som vandførende lag i lavpermeable morænelersaflejringer og formodes derfor at have stor betydning for den hydrauliske konduktivitet og transport i disse aflejringer. I denne afhandling er forekomsten, geometrien og sammenhængen af sandlinser i moræneler undersøgt med henblik på at vurdere indflydelsen på transporten af forureninger i lavpermeable aflejringer.

Sandlinser betragtes som enigmatiske geologiske indslag i glaciale sedimenter og er aflejret i et komplekst sammenspil mellem glacial aflejring og glacial tektonisk deformation. De subglaciale hydrauliske forhold og deformationsskræfterne er derfor bestemmende for udseendet af sandlinserne. På trods af hyppigheden og den forskelligartede tilstedeværelse, findes der kun sparsom information om sandlinser i litteraturen. For eksempel findes der ikke nogen konsistent terminologi for forskellige sand- og grusaflejringer i moræneaflejringer. I dette studie er den specifikke geometri af sandlinser karakteriseret gennem et feltstudium. Et antal geometriske parametre (længde, mægtighed, anisotropi, udbredelsesretning, osv) blev udvalgt til at beskrive størrelse og form af disse geologiske indslag. De karakteristiske træk blev benyttet til at definere et klassificeringssystem, der beskriver fem typer af sandlinser. Disse er: sandlag, sandtæpper, sandlegemer, sandlommer og sandbånd. Klassificeringssystemet er et nyttigt værktøj til at inkludere sandlinser i fremtidige morænelersundersøgelser, og det muliggør en hurtig klassifikation af morænelerstyper.

Den rumlige udbredelse af sandlinser er meget varierende på grund af den generelt komplekse lagfølge i moræneler. Samtidig er det en relevant parameter at beskrive, da middellængde og -afstand bestemmer sammenhængen mellem sandlinser. Pixelbaseret kortlægning af geologiske tværsnit blev i undersøgelsen brugt til at foretage en geostatistisk analyse. Variogrammer indikerede ikke-stationære strukturer, såsom vertikale trends, variabilitet i størrelse og stærk geometrisk anisotropi. Ikke-stationære strukturer komplicerede især identifikationen af korrelationsfunktioner og vanskeliggjorde simuleringen af fordelingen af facies. Transition probability-based geostatistisk modellering blev endvidere benyttet til at simulere udbredelsen af sandlinser og viste sig at være anvendelig til modelleringen af komplekse facies

opbygninger. Imidlertid viste multiple-point statistik bedre evne til at reproducere uregelmæssige geologiske strukturer. Især stærk anisotropi og variation i størrelse af sandlinser var bedst repræsenteret ved multiple-point simuleringer. Geostatistisk modellering af sandlinser muliggør identifikation af sammenhængen af sandlinser og kan blive brugt til at simulere heterogeniteten på ringe eller ikke undersøgte lokaliteter.

Når de specifikke strukturer af sandlinser er reproduceret på tilfredsstillende vis, kan hydrauliske parameter bestemmes for forskellige geologiske lag. Den gennemsnitlige hydrauliske konduktivitet for henholdsvis sandlinser og morænelermatricen varierer med tre til fire størrelsesordener. Sandlinsernes indflydelse på transporten vil derfor primært afhænge af forbindelsen mellem sandlinser. Tre-dimensionel visualisering indikerede forbundne netværk, hvorimod to-dimensionel modellering kun viste en begrænset forbindelse. Dette er et vigtigt aspekt for sandlinser, eftersom det understreger behovet for at samle data og efterfølgende repræsentere denne heterogenitet i 3D. Den fysiske betydning af sandlinsers heterogenitet blev undersøgt ved transportsimuleringer, som skulle efterligne forureningsspredning fra en morænelerslokalitet. Disse understregede behovet for at inkludere geologisk heterogenitet selv på lille skala. Sammenlignet med brug af gennemsnitligt eller tilfældigt varierende hydraulisk ledningsevne øgedes den horisontale spredning af forureningsstoffer, uden at den hydrauliske ledningsevne i morænelersaflejringer var øget i betydelig grad.

Sandlinser optræder i alle typer af glaciale sedimenter med varierende udbredelse og hydrauliske egenskaber. Geometrisk karakterisering har muliggjort klassifikation af de mest almindelige typer af sandlinser. Den geostatistisk analyse antyder, at sandlinser i moræneler skaber forbundne netværk især ved modellering i 3D. Som følge heraf er sandlinser vigtige i forbindelse med transport af forureninger i moræneler, og det anbefales derfor at inkludere heterogeniteten af sandlinser i risikovurderinger af forureningsspredning på morænelerslokaliteter.

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1 INTRODUCTION

1.1 MOTIVATION

Groundwater is worldwide an important source of drinking water, but contamination of various origin represents risk of leaching to aquifers (e.g. Gerke and Köhne [2004], Trolldborg et al. [2008], Chambon et al. [2010]). Potential sources are accidental spills from industrial sites and distributed application of agricultural chemicals. In North America and Europe many contaminated sites occur in areas with low-permeability fractured media [Parker et al., 1994, Christiansen et al., 2008, Chambon et al., 2011]. Contaminants have the tendency to infiltrate into the subsurface and migrate vertically along preferential flow paths [Nilsson et al., 2001, Jørgensen et al., 2002, Rosenbom et al., 2009]. Common contaminants are chlorinated solvents (PCE, TCE, VC) that are classified as dense non-aqueous phase liquids [Villaume, 1985]. Contaminated sites create groundwater plumes with high contaminant concentrations and large spatial extents. Transport and subsurface travel paths are determined by the hydraulic conductivity field and particularly by geological heterogeneities. The latter create preferential flow and comprise fractures, fissures, macro pores and lenses of coarse material.

The knowledge of relevant heterogeneity (e.g. fracture distribution) at contaminated sites is crucial to perform risk assessment and remediation technologies. Risk assessment tools consider heterogeneity usually with equivalent porous media (EPM) [McKay et al., 1997, Jørgensen et al., 2004b]. In the case of fractures, Jørgensen et al. [1998] and Sidle et al. [1998] showed that EPM models are insufficient to describe fracture heterogeneity and that discrete fracture models (DF) are favoured on short time scales. Detailed heterogeneity descriptions are also demanded for remediation design. Bioremediation as a naturally occurring process in the subsurface has been developed for technical application to clean up contaminated sites [Scow and Hicks, 2005, Aulenta et al., 2006, Manoli et al., 2012]. Dechlorinating microbial cultures and remediation amendments are injected into a system resulting in an enhanced *in-situ* degradation of contaminants. The delivery methods require spreading of the reactants and are thus dependent on conductive pathways within porous media [Christiansen et al., 2010]. In low-permeability sediments, the inclusion of heterogeneity is most important because it controls the advective transport in addition to the relatively slow diffusion.

The surface geology in large parts of the Northern hemisphere is dominated by glacial sediments [Houmark-Nielsen, 2003, 2010]. They are characterized as low-permeability sediments that are perhaps more variable than any sediments known by a single name [Flint and Davis, 1957]. Tills are fractured and interspersed with lenses of sand and gravel at multiple scales [Klint, 2001]. Fractures appear as elongated macropores and permeable lenses form hydraulic avenues within the till matrix. Both are believed to influence the transport behaviour of tills. Fractures have been described in numerous field studies [McKay and Fredericia, 1995, Jakobsen and Klint, 1999, Klint and Gravesen, 1999, Klint, 2001]. Less attention has been directed towards characterizing sand lenses in tills. Sand lenses occur in greater depths of till successions and may appear less important for the immediate migration of contaminants. However, they connect sub-vertical fractures and may shortcut the protecting till units above deeper aquifers. Sand lenses have been observed at numerous till sites (e.g. Krüger [1979], Phillips et al. [2007], Alexanderson [2010], Lesemann et al. [2010]), but consistent descriptions of geometry, properties or variability are not documented in the literature. Neither have sand lenses been classified respecting genesis, scale or hydraulic properties.

This study addresses this gap doing an in-depth investigation of sand lenses incorporated in clayey till successions. Hydrogeological modeling requires knowledge of flow paths, conceptual understanding of geological heterogeneity and not least the availability of high-resolution datasets. Given a known till stratigraphy and a full-scale characterization of sand lens heterogeneity, solute transport models for contaminated sites in clayey tills can be significantly improved. In many applications such models build the basis for risk assessment and are eventually used to support the design of remediation technologies.

1.2 OBJECTIVES

The overall aim of the PhD project is to characterize sand lenses in clayey tills and to assess the hydraulic impact of small-scale heterogeneity in low-permeability aquitards. The characterization includes genetic interpretations, geometrical descriptions and analyses of spatial variability. It is of primary interest whether or not sand lenses alter the equivalent permeability of tills and if connected sand lens networks facilitate preferential flow. The study of sand lenses contributes to the general understanding of geological heterogeneity in glacial sediments and gives suggestions on how to treat sand lenses when modeling transport processes.

The specific objectives are:

- Development of a field approach to characterize the geometry and shape of sand lenses at multiple scales. This includes mapping techniques on geological profiles and analysis of one dimensional borehole data.
- Introduction of a classification scheme for sand lenses that can be used to categorize sand lenses and relate them to till types. It builds on a field study collecting and interpreting sand lens data from till sites in Denmark.
- Characterization of spatial variability of sand lenses in till settings using geo-statistical tools. With regard to the hydraulic impact, the frequency, spacing, connectivity and spatial trend represent important criteria to investigate.
- Stochastic modeling of sand lens distribution with traditional two-point and multiple-point approaches. Emphasis lies on the evaluation of specific capabilities to reproduce complex shapes and non-stationary patterns of sand lenses.
- Performance of solute transport modeling including random-generated and simulated heterogeneity fields. The aim is to illustrate the effect of sand lenses on solute transport at a contaminated clayey till site in Denmark.

1.3 RESEARCH APPROACH

The PhD project follows a holistic approach, combining geological investigations in the field, geostatistical data analysis, stochastic simulation and hydrogeological modeling applications. The ambition to model solute transport at a contaminated site including a conceptualization of sand lens heterogeneity requires data collection at an analogue site Fig. 1.1. The Vadsby site has a contaminant source zone resulting from a spill of chlorinated solvents. Monitoring wells have been installed surrounding the source zone to determine hydraulic parameters and to determine the flow field. Geological data is restricted to borehole logs and stratigraphic models at site scale.

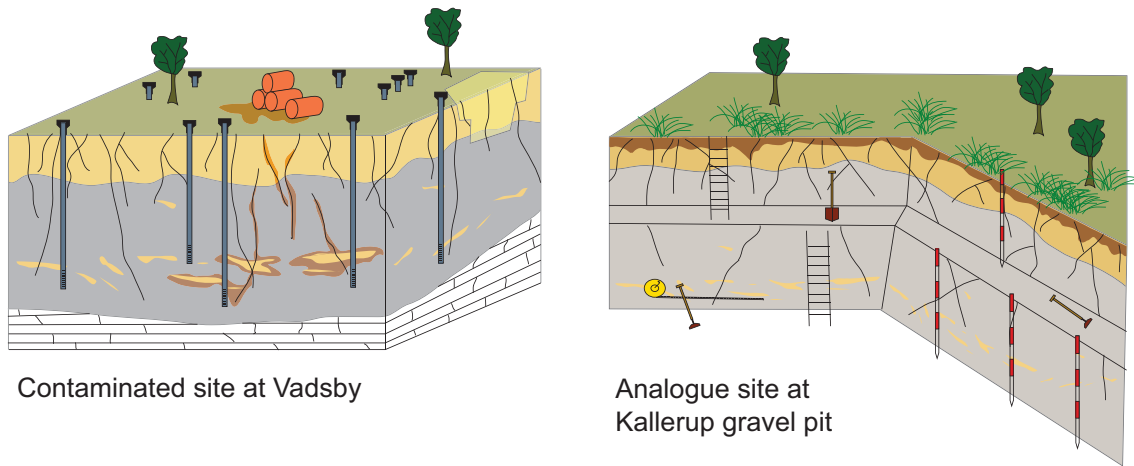


Figure 1.1: Conceptual model of clayey till sites. The left image shows the Vadsby contaminated site with boreholes and a point source and the right image the Kallerup analogue site with sand lenses exposed on a vertical outcrops. The analogue site serves to study and measure sand lenses in tills that is essential knowledge to characterize the transport paths at sparsely sampled sites.

The Kallerup gravel pit is located 1.5 km distance from the Vadsby contaminated site and exposes geological profiles of the entire till succession. Sand lenses were measured and mapped on excavated cross-sections that build the basis for the classification of lens types in clayey tills. The cross-sections were digitalized and transformed into training data to enable stochastic simulation of sand lens distribution. Two methods were selected for simulation, a transition probability-based algorithm and a multiple-point algorithm. Selected realizations were finally incorporated into a transport model of the Vadsby site. Several geological scenarios and hydraulic conductivity fields were tested and compared in terms of spreading and leaching of contaminants towards the underlying aquifers.

1.4 ORGANIZATION OF PHD STUDY

The study covers three different fields of research. The investigation of glacial geology and related heterogeneity was carried out in several field campaigns collecting geological data and interpreting observations. Paper I introduces delivery methods of remediation reactants to clayey till soils. The contribution includes the description of geology, identification of till types and measurements of fractures and sand lenses during excavations at the Vadsby site. More abundant sand lenses were found in an open pit in Kallerup promoting a detailed study of sand lenses occurring in greater depths. A methodology for systematic sand lens characterization including field examples is presented in paper II. The second activity includes geostatistical analyses and stochastic modeling applications. This was partly done in collaboration with a research group at the University of Neuchâtel and the results and evaluation of different simulation tools are summarized in paper III. The last step to characterize the hydrogeology of tills was done by means of modeling solute transport for a contaminated site. Results and findings are found in the technical note (IV).

The thesis itself is structured as follows. The first part of the thesis (chapters 2-6) is written as a synopsis of the work performed during the PhD. It contains an evaluation of the important findings and the applied methods and frames the individual contributions into a scientific perspective within the field of glacial geology and hydrogeology. In chapter 8 the scientific articles are presented in the form they were submitted for publication.

2 GLACIAL GEOLOGY

The late Pleistocene glaciations covered the Northern hemisphere including Scandinavia with a thick ice sheet. In Europe the latest glaciation period is referred to as the Weichselian glaciation and extended in the South to Germany and Poland and in the West to the British Islands [Houmark-Nielsen, 2003]. The footprints of the glaciation and the depositional history can be retraced interpreting glacial landforms and sediment successions [Bennett and Glasser, 2009]. In Scandinavia and particularly in the Eastern part of Denmark glacial deposits from this last main ice advance dominate the geology of the uppermost soil horizons [Houmark-Nielsen, 2007, 2010].

From a tectonic perspective, glaciations are an extremely dynamic period. Depending on the climatic conditions the ice mass is expanding or shrinking and is thus in constant motion. The weight of the ice leads to enormous pressures applied to the underlying bedrock and sediments [Bennett and Glasser, 2009]. Material is eroded, transported along with the ice flow and finally sedimented through lodgement or meltwater deposition [Evans, 2003, Bennett and Glasser, 2009]. These processes occur in different areas of a glacier and with varying intensity. Erosion occurs predominantly underneath the ice, whereas debris and melt-out material accumulate and deposit in the supraglacial and proglacial environment. Glaciotectonic deformation is further signing and altering the geological imprints [Hicock and Dreimanis, 1985, Hart and Boulton, 1991, Hart and Roberts, 1994]. Sediments are constantly deformed by compression, shearing or thrusting. Deformation occurs subglacially at the ice-bed interface and in the deforming layer beneath the ice [Hart, 1995, Tulaczyk et al., 2001, Rose and Hart, 2008]. Near the glacier margin sediments become folded or faulted and form push moraines [Hart, 1990, Phillips et al., 2008]. The deposition of heterogeneous material in combination with different styles and degrees of deformation leads to a unique and complex geology in glacial landscapes. Paying tribute to the degree of heterogeneity, glacial sediments are also called glacial diamictons or tills.

2.1 TILL CHARACTERISTICS

Deposition and deformation are recurrent processes and the sediments build till successions rather than homogeneous sedimentary units. There are different approaches to classify tills respecting genesis, style of deformation and geological features [Boulton and Deynoux, 1981, Dreimanis, 1989, Evans et al., 2006, Menzies et al., 2006]. The important till types and related characteristics are summarized in Tab. 2.1. There is ongoing discussion on the criteria to distinguish till types, particularly in the continuum between deformation till and lodgement till [Boulton and Deynoux, 1981, Benn and Evans, 1996, Ruszczynska-Szenajch, 2001, Evans et al., 2006]. With regard to sand lenses the term basal till is preferred for lodgement and deformation tills because both types experienced remarkable subglacial deformation [Benn and Evans, 1996]. On the other hand, it is important to distinguish between type A and type B tills [Evans et al., 2006, Kessler et al., II.]. The hydraulic regime determines the deformation style and thus the resulting structures and their specific shapes and forms [Lachniet et al., 2001, Larsen et al., 2007, Hart et al., 2011]. Type A denotes brittle deformation in a usually under-saturated bed and deformation of type B indicates a state with high water pressures and predominantly ductile deformation [Bennett and Glasser, 2009].

Tills are identified studying the local deposition history and measuring directional elements (clast fabric, scour marks, fold and fracture orientation) and textural soil properties [Berthelsen, 1978, Hicock and Dreimanis, 1985, Klint, 2001, Kjær et al., 2003]. These parameters are widely accepted and are as such crucial elements of till investigations. Less attention was directed to soft-sediment deformation structures such as sand lenses. These indicators are more complex to describe and contain more implicit information than directional elements. The correct interpretation, however, yields valuable inferences on depositional processes and events [Mills, 1983].

Table 2.1: Till types found in glacial landscapes. The table provides an overview of different types of glacial sediments with textural properties and deformation structures. It includes fractures and sand lenses as separate indicators to emphasize the link to related till types. The table is modified after a scheme of sedimentary characteristics presented in Bennett and Glasser [2009] and Kessler et al. [II.].

Till type	Structure / soil strength	Fabric signature / deformation style	Grain composition	Clast fabric / scour	Fractures	Sand lenses	Examples
Basal till	type B	low-medium strength; massive matrix	ductile shear; primarily folds or drag-folds	variable, but well mixed; ploughing clasts	medium/strong fabric	water-escape structures; hydrofractures	Kallerup [Kessler et al., II.]
	type A	high strength; dilatant, massive till	brittle and fissile shear zones; faults and thrusts	all grain sizes in fine grained matrix	very strong fabric along shear direction; high-angle clasts	systematic first order fractures	Breidamerkurjökull [Benn, 1995]
Glacietectonite	type B	medium strength; brecciated	non-penetrative deformation; pervasive, ductile shear; low cumulative strains	fine-grained matrix with clasts; boulder pavements	strong fabric parallel to local ice flow	-	Feggekliit [Pedersen, 1996]
	type A	medium to high strength; brecciated; foliated	penetrative deformation; brittle shear and localized ductile shear; tectonic foliation	fine-grained matrix with clasts; boulder pavements	strong fabric parallel to local ice flow	minor fracturing	Loch Lomond [Benn and Evans, 1996]
Flow till	low strength; poorly consolidated	chaotic structure; layers of fine material; stacked debris-flow packages	coarse and unimodal sizes; crude sorting; sorted pockets	angular shape; variable clast fabric; packages with strong fabric	minor fracturing	variables lenses of sand and gravel; varying sizes	Flakkebjerg [Klint and Gravesen, 1999]
Melt-out till	subglacial	low strength; unconsolidated matrix	massive; random oriented flow and fold structures; crude stratification	bimodal or multimodal sizes; similar to basal tills	striated, rounded clasts; strong fabric patterns from basal transport	few systematic fractures	Iceland [Klint et al., 2010]
	supraglacial	low strength; poorly consolidated matrix	massive; sedimentary structures; crude bedding in places; sorted and unsorted	coarse and unimodal sizes; abundant erratics	variable fabric; independent from ice flow	no tectonic fractures	Iceland [Klint et al., 2010]
Drop-till	moderate consolidated; laminated structure	weak deformation	very fine, silty/sandy sediments; clay-rich; dropstones in places	random fabric	no tectonic fractures	larger bodies or layers of fine sand; randomly deformed	Ontario, Canada [Klint, 1996]

2.1.1 FRACTURES

Fractures and sand lenses are common deformation structures in tills [McKay and Fredericia, 1995, Klint, 2001] and with regard to transport paths important heterogeneity. They are both effective as hydraulic avenues within low-permeability till matrices [Keller et al., 1988, Fredericia, 1990]. Fractures in glacial sediments have been described in a number of field studies, e.g. in McKay and Fredericia [1995], Jakobsen and Klint [1999] and Klint and Gravesen [1999]. In addition, hydraulically induced fractures were measured in Murdoch and Slack [2002] and Christiansen et al. [2008].

Klint and Gravesen [1999] showed that many factors are reflecting or influencing the fracture distribution in glacial deposits. Parameters to describe fractures include the spacing in vertical and horizontal direction, the orientations in form of the dip and strike and the mean apertures [McKay et al., 1993, Klint and Gravesen, 1999]. Klint [2001] introduced a systematic methodology to describe and categorize fractures in tills. The scheme is a useful tool to link fracture observations to till types and to develop an additional indicator to identify glacitectonic deformation processes.

2.1.2 SAND LENSES

Along with fractures, sand deposits have been observed in numerous till studies [Krüger, 1979, McCabe, 1987, Clayton et al., 1989, Lønne, 1995, Krüger, 1997, Kjær et al., 2004, Alexanderson, 2010]. They were described as sand lenses, interbedded sands, sand stringers and similar denotative terms. However, no consistent nomenclature with characteristic properties for different types is documented in the literature. The aim to include sand lenses when describing geological heterogeneity in tills makes a consistent and systematic characterization of sand lenses essential. Oriented at the methodology for fracture classification, a similar approach was developed for sand lenses in Kessler et al. [II.]. The framework of this particular study was to measure sand deposits occurring in glacial sediments and to interpret and categorize them according to their genetic, geometric and structural characteristics. The understanding of formation and alteration processes of sand lenses in tills is hereby fundamental to enable plausible classification.

Sand lenses are the result of a complex interplay of glacial deposition and deformation [Evans et al., 2006, Bennett and Glasser, 2009]. The dominant processes in the different glacial environments are summarized in Kessler et al. [II.] and illustrated in Fig. 2.1. Debris accumulates on the glacier surface and becomes displaced and sedimented near the glacier margin. It typically creates a chaotic and heterogeneous mélange of supraglacial material that includes sand and gravel features. The microstructures in such flow deposits have been described in Bertran and Texier [1999], Menzies and Zaniewski [2003] and Phillips [2006]. Similar coarse-grained debris deposits that are larger in extent form during back- and down-wasting of melting ice in dead-ice landscapes [Paul and Eyles, 1990]. Examples are reported from the Kötlujökull glacier in Iceland [Krüger, 1997, Kjær and Krüger, 2001]. A major source of sorted sand deposits in tills are meltwater sediments deposited by fluvial, lacustrine or even marine sedimentation. They form channel shaped or extended sand and gravel plains and have been documented in a broad range of studies from numerous sites in Scandinavia and North America (e.g. Anderson [1989], Sharpe and Cowan [1990], Sadolin et al. [1997], Eyles [2006], Goutaland et al. [2008]). Important representatives of meltwater sediments are proglacial sandur deposits and outwash fans [Evans, 2000, Kjær et al., 2004, Krüger, 1997], lacustrine deposits from glacier surges [Russell et al., 2001, Larsen et al., 2006, Benediktsson et al., 2009] and subglacial sediments originating from ice-bed decoupling events [Piotrowski et al., 2006, Lesemann et al., 2010]. Waterlain sediments are closely related and build fine-grained and sorted sandy or silty sediment layers [Krzyszkowski and Zielinski, 2002].

Once deposited, sandy and gravelly deposits undergo permanent glaciotectionic deformation by recurrent glacier advances [Hart and Boulton, 1991, Benn and Evans, 1996]. Shear and other frictional forces underneath the glacier dislocate and reshape sediments and alter their constitution [Aber, 1982, Hart and Roberts, 1994, Jakobsen, 1996, Pedersen, 1996]. Glaciotectionic deformation eventually forms the characteristic till sediments, but at the same time creates smaller lenses of coarse-grained or sandy material. These result from mainly ductile deformation during high-pressurized hydraulic regimes. Hart and Roberts [1994] and Piotrowski et al. [2006] describe the process of sediment folding in the deforming layer creating attenuated lenses and boudinages that migrate into the overlying till. The resulting elongated and anisotropic lenses are typically found in flow tills and immature basal tills [Kessler et al., II.]. Sand intrusions were characterized as macro pores and small cavities that become filled with fine sands, due to high water pressures

in the bed [Jolly and Lonergan, 2002, James et al., 2003]. In contrast, brittle deformation in under-saturated systems leads to faulting and small-scale thrusting in the deforming bed [Benn, 1995, Benn and Evans, 1996]. Larger thrust complexes and related facies architecture in glacier-marginal environments have been studied in Denmark in Klint and Pedersen [1995] Pedersen [2005].

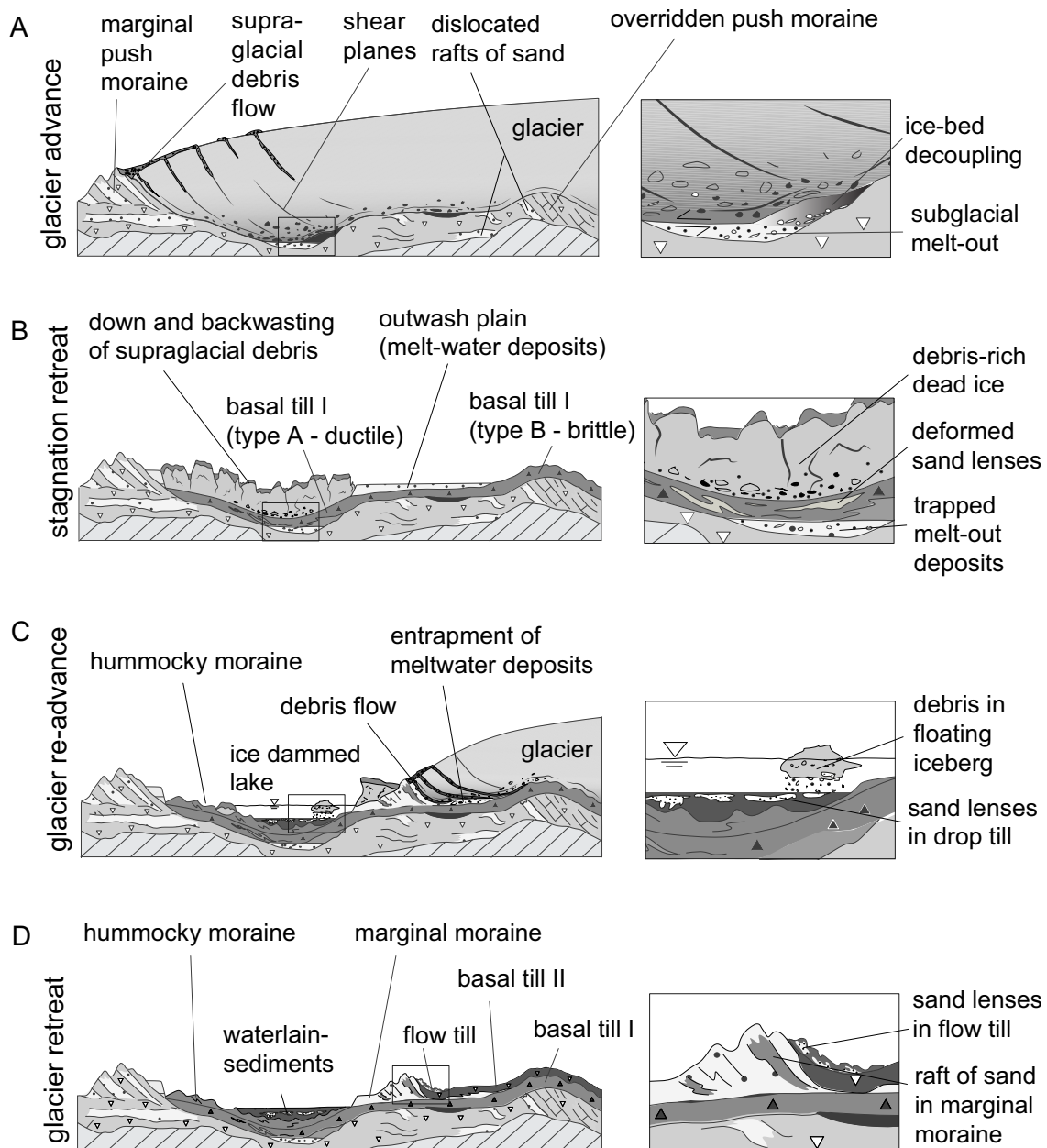


Figure 2.1: Illustration of glacial deposition and deformation processes. Images A to D illustrate a glacial cycle from the first advance to the final retreat. The processes leading to the deposition and formation of sand lenses are highlighted in the small figures on the right side of the figure. The illustration is modified after Houmark-Nielsen et al. [2005]

2.2 CLASSIFICATION OF SAND LENSES

The process understanding of sand lens genesis is a first step to characterize till heterogeneity. The second step is to conceptualize sand lens types and to allocate them to classes with specific geometric and physical properties. The diversity of processes forming and deforming sand lenses challenges such schematization. It requires field measurements at multiple scales combined with genetic interpretations. In Kessler et al. [II.] sand lenses were parameterized in terms of geometry, composition and internal architecture. The parameters with the largest variability were used to circumscribe classes of sand deposits. These are the extent in horizontal and vertical direction, the anisotropy ratio, the frequency and the degree of deformation. Minor aspects regard the grain composition, the orientation or the sedimentary structures within sand deposits.

The presented classification scheme in Kessler et al. [II.] yields five different classes of sand lenses. These are likely not sufficient to encompass all types of sand lenses, but they mark a starting point to systematize sand lenses in tills. The largest structures are defined as sand layers and decreasing in spatial extent follow sand sheets, sand bodies, sand pockets and sand stringers (Fig. 2.2). Sand layers occur in between till transitions and are deposited by meltwater sedimentation, primarily in the proglacial environment. Thinned and elongated features incorporated in the till matrix are the result of sub-horizontal shear deformation in the deforming layer of the sediment. Typical representatives are sand sheets with anisotropy ratios of >50 . Sand bodies are thicker than sheets, have heterogeneous shapes and show mixed sedimentary or sorted internal structures. They form from debris flow and fluvial deposition and become reworked by re-advancing glaciers. The abundant sand pockets are associated with boudinages or attenuated folds. They become dislocated from larger deposits and migrate into the till matrix. Sand stringers are the smallest features with only a few centimeters thickness. They typically depict deformation structures and directions nicely.

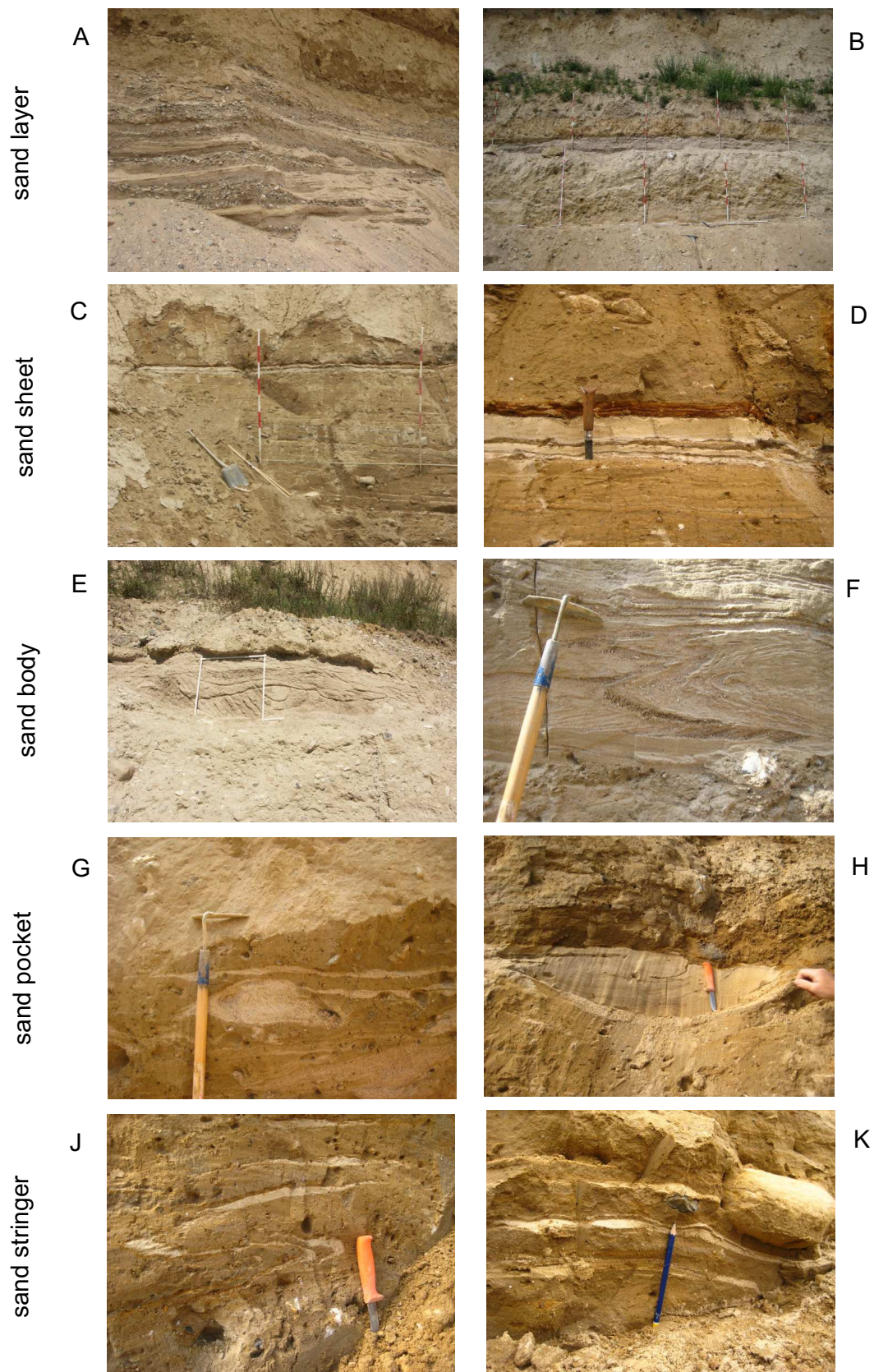


Figure 2.2: Images of sand lenses. The series shows examples of the sand lenses according the defined classes. From top to down these are sorted from large deposits to smallest features: sand layers, sand sheets, sand bodies, sand pockets and sand stringers.

2.3 FINDINGS FOR SAND LENSES

The introduced methodology on characterizing, parameterizing and classifying sand lenses is an attempt to include sand lenses in till investigations. Sand lenses are recognized in numerous till types and can be used for till identification and description. Sand lenses are as such a supplemental criterion and need to be combined with traditional fabric measurements and micro-structural analyses. Besides, the classification further provides a guideline to accurately name sand lenses respecting the form of appearance and genesis in a glacial framework.

3 HETEROGENEITY IN CLAYEY TILLS

Studies of geological heterogeneity received increasing importance because of abundant problems regarding subsurface transport of fluids and contaminants [Koltermann and Gorelick, 1996, Gomez-Hernandez and Wen, 1998, Zinn and Harvey, 2003, Feyen and Caers, 2006, Michael et al., 2010]. The aim was to describe property fields of hydraulic conductivity or porosity at the local and regional scale. The limitation to describe these parameters is a global lack of data of the subsurface. Characterization of hydraulic properties in glacial diamictons are especially challenging, due to the specific transport framework and complexity of heterogeneity in such settings [Ritzi et al., 1994]. Transport is controlled by preferential flow occurring in macro pores or coarse-grained sediment facies [McKay et al., 1993, Nilsson et al., 2001, Jørgensen et al., 2002]. Additional complexity is caused by striation, sorting, lineation or anisotropic arrangement of fabric. Against this background, Anderson [1989] stated that heterogeneity models need to represent the geometry and architecture of interconnected high-permeability facies or flow paths. Characterization thus emphasizes on geological structure rather than on hydraulic properties distribution. Jørgensen et al. [2002], LeBorgne et al. [2006], LeBorgne et al. [2007] and Bianchi et al. [2011] present such approaches identifying preferential flow paths in heterogeneous settings. Applied to clayey tills this means to focus on the description of size, shape, distribution and connectivity of fractures and sand or gravel lenses.

3.1 CHARACTERIZATION METHODS

Firstly, concepts and strategies to enable extensive data collection of the subsurface need to be developed for field application. In a second step, geostatistical modeling tools can be employed to parameterize and to simulate sand lens variability at locations where dense sampling is unfeasible. Sand lenses have diverse forms of appearance, occur in varying depths and on multiple scales [Kessler et al., II.]. Therefore, a single-best approach for its characterization is not existent. Depending on the location, scale and variability of features, a combination of methods is recommended to assure high data quality and good interpretability. The different characterization methods are outlined in the following Tab. 3.1.

Table 3.1: Methods to characterize geological heterogeneity. They are distinguished in terms of data type, sampling method, dimension, scale and data quality. Examples of documented characterization of heterogeneity in clayey tills are given in the last column.

Character-ization method	Data type	Sampling method	Dimension / Extent	Scale / Resolution	Data quality	Examples
Borehole logging	hard data, facies successions	invasive drilling or coring	1D transects, bordered at bedrock surface	few cm to 10s of meters	++	
Outcrop mapping	hard data, geological descriptions, drawings, digital imaging	clearing natural cliffs	2D outcrops, limited by topography	few dm to hundreds of meters	++	Sjørring et al. [1981], Pedersen [2005]
Excavations	hard data, geological descriptions, drawings, digital imaging	invasive digging and slicing	pseudo-3D, limited in depth (ca. 10m)	few mm to 10s of meters	+++	Christiansen et al. [2012], Kessler et al. [II.]
Geophysical surveys	soft data, indirect measurements (resistivity, etc.)	non-invasive airborne or surface mapping	2D and 3D, limited penetration depth	several dm to km, large resolution	+/- (depending on the method)	Kilner et al. [2005], Cuthbert et al. [2009]
Stochastic simulation	predictions, interpolations	simulation	all dimensions, numerical constraints	all scales, all resolutions	-/+ (depending on conditioning)	Ritzi et al. [2000], Comunian et al. [2011b]

3.1.1 BOREHOLE LOGS

Borehole logs from well drilling or coring are common data sources to resolve the sedimentary stratigraphy or the vertical sequence of geological facies. In Denmark, lithological data are recorded at reasonable sampling intervals and stored in an open access database called JUPITER [Tulstrup, 2004, Hansen and Pjetursson, 2011]. Borehole logs are one-dimensional and can hardly provide enough detail to characterize small-scale heterogeneity or sand lenses. Experiences from drillings in clayey tills have shown that smearing and mixing effects inside the borehole destroy the erosive contacts between sand and clay at the centimeter scale. In addition, the spacing of logs must not be much larger than the horizontal correlation length of lenses to capture the two-dimensional structure. Such dense sampling campaigns are generally unfeasible and borehole logs are considered deficient to describe sand lens heterogeneity.

3.1.2 NATURAL OUTCROPS

Natural outcrops allow mapping of complete, two-dimensional profiles at different scales and are an excellent geological data pool. Outcrops provide horizontal cuts of geological units where structures and sedimentary deformation features can be studied. There are a number of field examples in Denmark where glacial sediments and related heterogeneity (sand deposits, thrust planes, folds, etc.) were measured and mapped on exposed push ridges [Klint and Pedersen, 1995, Pedersen, 2005, Sjørring et al., 1981]. A major advantage of mapping outcrops is the variety of scales. Sand lenses at the centimeter scale can be captured equally well as large-scale thrusts or beds of sand in the range of tens of meters. Unfortunately, accessible outcrops are rare and limited to coastal cliffs and river valley. Investigations of geological heterogeneity within a specific horizon are therefore not always possible.

3.1.3 EXCAVATIONS

Excavations combine the advantages of the two previous methods. Vertical cross-sections are revealed at the site and in the geological unit of interest. It enables detailed insight into the heterogeneity at a specific location and offers access to the entire geological profile by slowly advancing into greater depths. Excavating the ground is limited in scale and depth and requires enormous logistical and economical efforts. Results from experimental sites to investigate fractures and sand lenses in tills are reported in Kessler et al. [II.] and Christiansen et al. [2012]. The greatest advantage of excavations is the flexibility when clearing excavated walls. The orientation as well as the height of the profiles can be determined facilitating the identification of anisotropic shapes or directional features. In practice, excavations have only minor importance as deep excavations are only performed in combination with remediation projects or construction activities, where limited or no access is permitted for geological investigations.

3.1.4 GEOPHYSICAL SURVEYS

Geophysical data are considered soft data because the measurable properties (electrical resistivity, dielectric permittivity, seismic velocity, etc.) are in a certain relation to physical or hydrogeological parameters (porosity, hydraulic conductivity,

lithology, etc.). Geophysical measurements are inexpensive, minimally invasive and provide large datasets with high sampling density. In Denmark, geophysical methods have been widely used to interpret the sedimentary geology of quaternary valleys and other glacial landforms [Jørgensen et al., 2003, Kilner et al., 2005, Cuthbert et al., 2009]. Geophysical measurements include significant degree of uncertainty, if they are interpreted separately. An integrated analysis of different data types reduces uncertainty and can enhance traditional geological investigations. Geophysical methods have proved useful to delineate lithological successions or to identify thick meltwater sequences. Small-scale geological features, however, are beyond the capabilities of such methods and need to be characterized by other means.



Figure 3.1: Characterization methods for geological heterogeneity. The pictured methods were employed in Denmark to record sand deposits in clayey tills. They are in particular: A borehole logging, B outcrop mapping, C excavations, D airborne geophysical surveys, and E stochastic simulation.

3.1.5 SIMULATION

Stochastic simulation is not considered as a separate geological characterization method. It is rather used to post-process or upscale existing datasets by estimating the realizations of a geological variable at unsampled locations. Simulation algorithms always require input of either true data, training images or at the minimum measures of spatial variability. After having examined spatial structures or patterns, the distribution of geological facies can be simulated at chosen scales and dimensions.

3.2 TILL ANALOGUES

Sand lenses typically occur in depths of 10 meters and more with dense clayey till units deposited on top. Most of the features have small thickness in the range of centimeters to decimeters [Kessler et al., II.]. As a result, none of the above mentioned characterization methods are solely appropriate to fully describe this type of heterogeneity at, for example, contaminated sites. Analogue studies bridge the accessibility and scaling limitations by investigating sites that expose sand lenses in corresponding geology. Gravel pits offer excellent opportunities to perform outcrops studies and detailed mapping exercises. Profiles at the edges of the pit display till successions and additional excavations in large depths are easy to realize (Fig. 3.2). To transfer heterogeneity to unsampled sites, geostatistical methods are employed. The parameterization of spatial variability enables simulations of facies geometry and architecture that are ideally conditioned with hard data from boreholes at the sites of interest. For sand lenses in tills, such an approach seems the only feasible alternative to represent fine-scale heterogeneity at sparsely or unsampled sites [Kessler et al., III.].



Figure 3.2: Excavation in the Kallerup gravel pit. The images show the Kallerup profile N and the excavation of smaller cross-sections. These were used to measure and map sand lenses at small scale.

In general, analogue studies are applicable if a) the geological stratigraphy of the analogue site is comparable, b) an accessible analogue site is available, and c) conditioning datasets exist from the site of interest. Given these conditions being fulfilled, analogue studies can significantly improve hydrogeological descriptions. It is hereby crucial to assess the uncertainty for each individual application, because conditioning data is often sparse and stochastic simulations estimate the realizations of geological variables. Analogue studies can be done in different geological settings and with different types of data involved. Bayer et al. [2011] and Felletti et al. [2006] performed analogue studies in fluvio-glacial aquifers using outcrop and/or geophysical data. A similar approach using geophysical lidar imaging was reported in Klise et al. [2009]. Alluvial settings with multiple hydrofacies as channel and interchannel deposits are a classical application and are reported from both, natural outcrops [Dai et al., 2005] and artificial or quarry outcrops [Falivene et al., 2006]. The common objective of all studies of heterogeneity including Kessler et al. [III.] is to obtain detailed representations of facies architecture and their specific connectivity patterns with regard to flow and transport paths in porous media.

3.2.1 DESCRIPTION OF SAND LENS GEOMETRY

Sand lenses are treated as a geological facies type as well as individual geobodies. The configuration in space as well as characteristic geometries are essential knowledge for a complete characterization. Excavated cross-sections ensure high-quality data collection and are suitable for geometric measurements and discrete mapping procedures (Fig. 3.3). It is recommended to investigate a number of equally-sized cross-sections with a minimum of 20 individual sand lenses. The dimension of the cross-sections should be chosen accordingly, but should be large enough to encompass the entire extent of larger sand bodies or sand sheets [Kessler et al., III.]. It is further recommended to excavate sections parallel and perpendicular to the deformation direction to capture horizontal anisotropy.

Field measurements include parameters such as length, thickness, dip angle and deformation structures, and require only simple measuring tools (scraper, knife, tape measure and a geological compass). The measurements can be taken on site or derived from photographs preserving the scale of the image. All relevant geometric parameters for the characterization of single sand lenses and mean values from field investigations are discussed in Kessler et al. [II.].

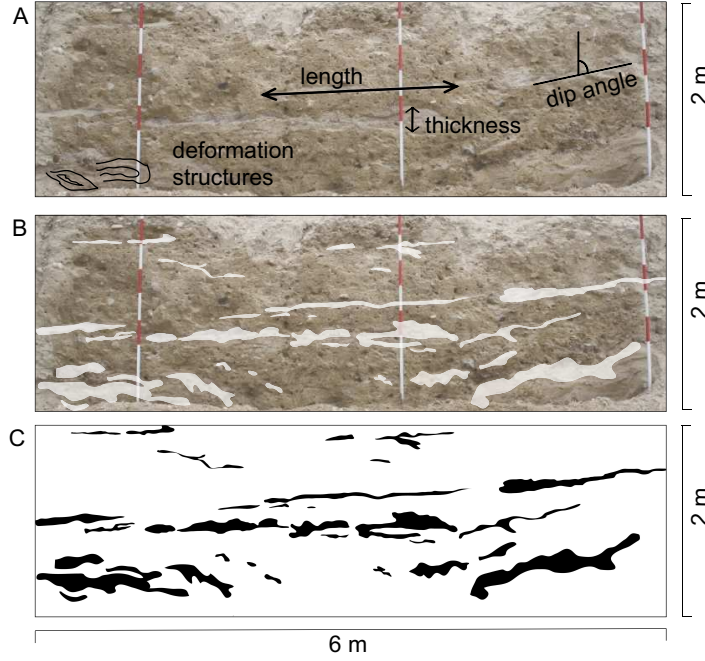


Figure 3.3: Illustration of the mapping procedure of sand lenses on geological outcrops. The three pictures show A cross-section with measuring sticks, B cross-section with sand lenses indicated, and C categorized image with two facies (clay and sand).

The majority of sand lenses are stringers and pockets in the centimeter to decimeter range. They have elongated shapes and vary primarily in extent and anisotropy [Kessler et al., II.]. The geometry can be approximated calculating the statistics of size, mean lengths in three directions and anisotropy ratios. Sand lenses are anisotropic if mean lengths differ with direction [Carle and Fogg, 1996]. The vertical anisotropy in x direction is defined in Equ. 3.1 with L_x and L_z denoting the length in horizontal and vertical direction.

$$(3.1) \quad a_v = L_x / L_z$$

3.2.2 ANALYSIS OF SPATIAL VARIABILITY

The spatial variability of sand lenses is recorded using photographic mapping techniques and transforming section images into numerical datasets (Fig. 3.3). Geostatistical analyses or variogram modeling is a common approach to determine parameters of correlation and to develop models of continuity [He et al., 2009]. First, the experimental variogram is computed from the digitalized section images and

then, a mathematical model is fitted to the values [Webster and Oliver, 2007]. The model eventually yields the measures of spatial correlation like the range (plural if nested models), the sill and potential nugget effects. The variogram is defined as follows:

$$(3.2) \quad 2\gamma(\mathbf{h}) = E \left[\{Z(\mathbf{x}) - Z(\mathbf{x} + \mathbf{h})\}^2 \right]$$

In modeling the variogram, a common assumption is that features are Gaussian or randomly distributed within a defined domain. Lithological maps of till outcrops reveal that sand lenses rarely have this property. Sand lenses occur close to geological transition or thrust planes meaning that they concentrate in certain areas of a cross-section and show spatial trends. In addition, varying feature sizes, periodicity and anisotropy complicate the parameterization of spatial variability. In geostatistical terms this phenomenon is referred to non-stationarity. In Fig. 3.4 exemplary variograms in horizontal and vertical direction are shown for sand lenses on two chosen till cross-sections.

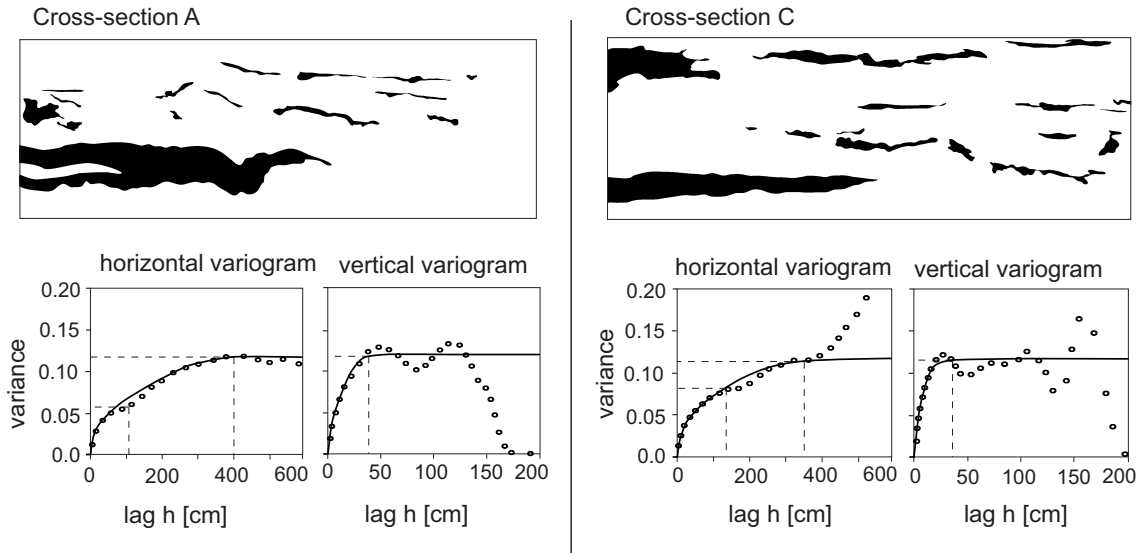


Figure 3.4: Example of analysis of spatial variability on till cross-sections. The upper images show categorized till cross-sections with sand lenses indicated in black color. The lower graphs show the variograms for both sections in horizontal and vertical direction. The experimental variogram is plotted with little circles and the solid line shows the modeled variogram. The dashed lines mark the sill and range for each of the nested structures.

3.3 FINDINGS FOR TILL HETEROGENEITY

Compared to the distribution of hydrofacies in alluvial aquifers, sand lens heterogeneity in tills occurs at smaller scales with an increased degree of complexity in terms of geometry and distribution. Sand lenses have elongated, anisotropic shapes with horizontal extents ranging from few decimeters to tens of meters. They show spatial trends towards till transitions and have multiple non-stationary properties. Outcrop studies performed at analogue sites are considered the most appropriate method to capture the nature of sand lens variability. Field measurements and mapping procedures are easy to perform on vertical outcrops and correlation measures required for simulation are most precise if inferred from complete digital section images.

4 SIMULATION OF SAND LENSES

Field characterization of geological heterogeneity can never be certain, continuous and complete for the entire modeling domain. This may be due to sparse data (borehole logs), uncertainty of data (geophysics) or inaccessibility of relevant sites (outcrop studies). These constraints call for methods to parameterize collected data in order to complete patchy descriptions or to transfer knowledge to external sites. Geostatistics offer such opportunities as interpolating geological variables between sampled locations or predicting realizations of variables at unsampled sites [Webster and Oliver, 2007, Kitanidis, 1997]. Stochastic methods are particularly expedient for simulation. They require measures of spatial correlation and return, besides the simulated realizations, estimates of uncertainty [Webster and Oliver, 2007, Renard, 2007]. Geostatistics further allow incorporation of a broad range of data types (geological, geophysical or hydrological information) into simulations and to produce multiple realizations of the same variables [Koltermann and Gorelick, 1996].

4.1 ALGORITHMS AND APPLICATIONS

Stochastic methods first evolved in hydrogeology to generate property maps of hydraulic or soil parameters, e.g. hydraulic conductivity [Koltermann and Gorelick, 1996, Fogg et al., 1998, de Marsily et al., 1998]. Multi-Gaussian models were commonly used with the limitation of not being able to model a wide spatial range of patterns [Journel and Alabert, 1990, Gomez-Hernandez and Wen, 1998, Zinn and Harvey, 2003, Renard et al., 2005, Kerrou et al., 2008]. The way forward was to decompose the simulations into a two-step procedure, namely the simulation of lithofacies and subsequently to populate those with hydraulic or transport parameters [Renard, 2007, Mariethoz et al., 2009]. The evolving methods could be conditioned to hard, geological field data and become constrained with subjective geological knowledge of the internal facies architecture [Carle, 1996, Fogg et al., 1998, Renard, 2007].

In geological applications, data are mostly of categorical type (e.g. lithofacies codes) that are modeled with indicator methods. There are multiple indicator simulation algorithms available for problems where geological facies are identified from field observations [Koltermann and Gorelick, 1996, de Marsily et al., 2005].

Table 4.1: Simulation algorithms used for simulation of categorical variables in geological applications. The methods have been used to model the distribution of hydrofacies in numerous synthetic cases as well as in field applications. The table highlights the parameterization, advantages and limitations of the methods and lists a small number of field applications.

Algorithm	Spatial correlation measure	Parameters	Limitations	Advantages	References	Documented applications
Truncated Pluri-gaussian Simulation	variogram	sill, range, nugget	<ul style="list-style-type: none"> • facies need to be ordered • only one variogram model to describe spatial variability 	<ul style="list-style-type: none"> • respects relations between lithofacies • univariate simulations 	Matheron et al. [1987], LeLoch et al. [1994]	modeling sandstone analogue [Falivene et al., 2006]; clay-sand distribution [Mariethoz et al., 2009]
Boolean method	marked point processes		<ul style="list-style-type: none"> • difficult to constrain density of geobodies • limited capability to condition to dense, local data 	<ul style="list-style-type: none"> • produces realistic geometries 	Deutsch et al. [1992]	petroleum reservoir modeling e.g. Bratvold et al. [1995], Tyler et al. [1994]
Sequential Indicator Simulation (SIS)	indicator-variogram	still, range, nugget	<ul style="list-style-type: none"> • problem to simulate complex structures • consistency problems • unrealistic transitions 	<ul style="list-style-type: none"> • statistical parameters are easy to infer • robust algorithm 	Webster [1985], Goovaerts [1997]	modeling clay content [He et al., 2009]; hydrofacies distribution [Klise et al., 2009]
Transition Probability-based Statistics (TP)	transiogram	proportions, mean lengths, juxtapositions	<ul style="list-style-type: none"> • problems to simulate complex structures • parameterization limits variability 	<ul style="list-style-type: none"> • consideration of subjective geological knowledge • 3D variability characterized with 1D Markov chains • fast and robust algorithm 	Carle and Fogg [1997], Carle [1999]	facies in alluvial fans [Fogg et al., 1998, Weissmann et al., 1999]; glaciofluvial deposits [Proce et al., 2004, Kessler et al., III.]
Multiple-point Simulation (MPS)	search template	proportions, scale, anisotropy	<ul style="list-style-type: none"> • computationally demanding • requires training images in the same dimension 	<ul style="list-style-type: none"> • extremely flexible • facilitates conditioning • can model complex spatial relations between facies 	Strebel [2002], Liu et al. [2006], Straubhaar et al. [2011]	facies architecture in aquifers [Huysmans and Dassargues, 2009, Comunian et al., 2011b]; sand lenses [Kessler et al., III.]

They all have their strengths and weaknesses depending on the type of heterogeneity, the scale and the specific application (Tab. 4.1). The list of approaches focuses on pixel-based methods but we do recognize object-based methods as a valuable alternative for specific applications.

The first applications are reported from the petroleum industry modeling the spatial variability of oil reservoirs. Later, focus was shifted towards modeling connectivity patterns in porous media, e.g. the distribution of conductive lithofacies and the structure of macro pore networks, since they strongly control flow and transport [Zinn and Harvey, 2003, Knudby and Carrera, 2005, Kerrou et al., 2008, Bianchi et al., 2011]. The applications given in Tab. 4.1 are mostly performed at spatial scales of 10s to 100s of meters to model the internal architecture of aquifers. Particularly examples from alluvial or fluvial settings with three to four lithofacies are frequently documented in the literature (e.g. [Weissmann and Fogg, 1999, Felletti et al., 2006, Zappa et al., 2006, Lee et al., 2007, dell’Arciprete et al., 2011]). Minor attention was paid to model small-scale geological features and, besides the distribution of facies, to reproduce complex geometries of anisotropic heterogeneity.

The latter aspect gave rise to multiple-point statistics (MPS) that proved more flexible than traditional two-point methods [Caers and Zhang, 2002, Strebelle, 2002, Liu et al., 2006]. However, it has been applied mainly to synthetic cases to show the ability to simulate connectivity patterns [Feyen and Caers, 2006, Arpat and Caers, 2007]. A well-known example was published in Strebelle [2002], where an MPS model represents the distribution of a channel facie in a fluvial setting, but also reproduces the curvilinear pattern of channel structures (Fig. 4.1). This is an important improvement because geometry and connectivity may have an even larger impact on the transport properties compared to simple facies proportions implied by percolation theory [Stauffer and Aharony, 1994].

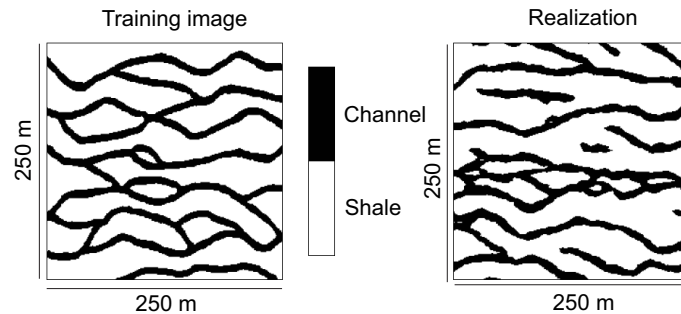


Figure 4.1: Illustration of an MPS application of a fluvial channel system. The connectivity of the channel structures on the training image is well reproduced on the realization. This example was first published in Strebelle [2002].

Huysmans and Dassargues [2009] and Comunian et al. [2011b] reported MPS applications modeling anisotropic hydrofacies heterogeneity in real aquifers. This approach emphasizing on the variability of geological structure was followed in Kessler et al. [III.] with an attempt to simulate fine scale and complex geological features, namely sand lenses in clayey tills. The enhanced capabilities of MPS to reproduce specific shapes of geobodies were tested by means of a comparison of two stochastic methods, a transition probability-based and multiple-point approach.

4.2 MODELING FINE SCALE STRUCTURES

According to the findings presented in Kessler et al. [II.], sand lenses have varying sizes and anisotropic shapes in all principal directions. They are thus a good example of geological structure occurring at multiple scales with non-stationary patterns including geometric anisotropy, spatial trends and periodicity (see Chapter 3.1). Most current simulation algorithms are challenged with non-stationary properties of facies [Bastante et al., 2008, Comunian et al., 2011a]. On the other hand, they facilitate critical performance assessment of different methods, particularly if fine scale and fully discretized data from mapped outcrops are available.

In Kessler et al. [III.] a modified approach of using outcrop data for simulation was introduced. Instead of reproducing observed or measured structures on two dimensional analogues [Falivene et al., 2006, Klise et al., 2009, Bayer et al., 2011, Comunian et al., 2011b], one cross-section was used to simulate a different, yet parallel section (Fig. 4.5). This approach is beneficial to study the potential of high resolution analogue data to simulate unsampled sites and to evaluate the effect of conditioning data. Hard geological data are generally available from a finite number of randomly distributed borehole logs. Vertical data columns of facies successions, mimicking wells or boreholes, can be used to condition simulations. Sand lenses in tills are best modeled as a simple two category system considering a) a low-permeability clayey matrix, and b) conductive sand lenses incorporated within the matrix [Kessler et al., III.].

4.2.1 TRANSITION PROBABILITY VS. MULTIPLE-POINT SIMULATION

Transition probability approach (TP) is based on one-dimensional Markov chain models and is a typical representative for two-point statistics. Unlike (cross-) variogram or covariance-based models, TP is implemented calculating the probability that two points separated by a certain lag distance have the same or a different value (see Equ. 4.1 and [Carle and Fogg, 1996, Carle, 1999]). The realization of a variable x is hereby only dependent on the nearest neighbor or the closest lag. The spatial correlation is parameterized with mean lengths and proportions that are derived from the Markov models illustrated with transiograms (Fig. 4.2). The parameterization with mean lengths yet hampers the simulation of geobodies with varying size and extent.

$$(4.1) \quad t_{jk}(\mathbf{h}) = \frac{E \{I_j(\mathbf{x})I_k(\mathbf{x} + \mathbf{h})\}}{E \{I_j(\mathbf{x})\}}$$

The strength of the TP method is the ability to link observable geological attributes to model parameters, and in this manner to account for more geological structure. This advantage is discussed in comparison with sequential Gaussian methods in Lee et al. [2007] and for sequential indicator methods in He et al. [2009]. Juxtapositional tendencies have proved useful for multi-categorical problems [Weissmann et al., 1999] but are of no importance to sand lens models [Carle and Fogg, 1996].

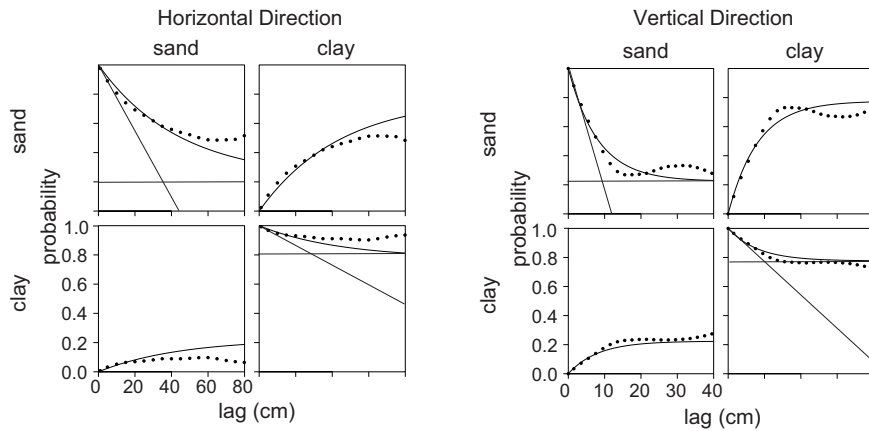


Figure 4.2: Transiograms of a mapped till section. The transition probabilities are calculated for all auto- and cross-transitions. The data is modeled with spatial Markov chains. The straight lines mark the approximate proportions (horizontal line) and the mean lengths in horizontal and downward direction (tangents at the origin of Markov models).

Multiple-point statistics disregard the spatial correlation between two points but investigate recurrence of specific spatial patterns. This is achieved scanning training images (TI) that are directly derived from outcrop maps. The principle of the method and the underlying algorithms are explained in Caers and Zhang [2002], Strebelle [2002] and Hu and Chugunova [2008] and briefly outlined in the flowchart in Fig. 4.3. The increased flexibility of MPS in terms of simulating anisotropic shapes and variably sized geobodies are traced back to specific search tree design and multigrid implementation [Liu, 2006, Remy et al., 2008]. Further, non-stationary patterns on cross-sections can be partially accounted for with subgrid and region concepts [Remy et al., 2008], which are not available for TP approaches.

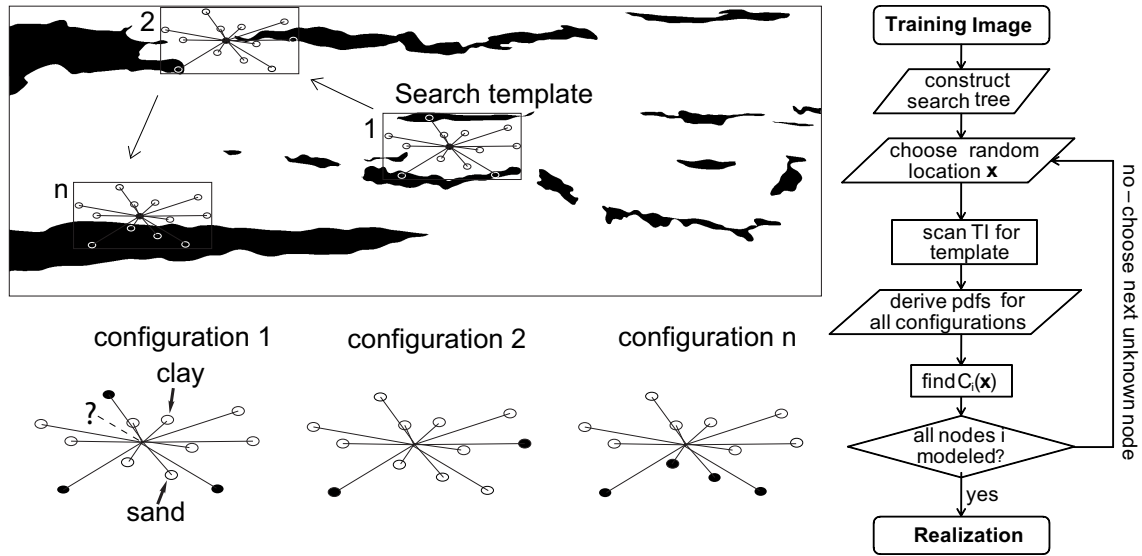


Figure 4.3: Illustration of multiple-point algorithm. The search template is defined as a random cluster of points in the neighborhood of a node (search tree). The TI is scanned for the search template at each node and a probability distribution is derived determining the realization at the simulated node.

4.2.2 FROM 2D TO 3D SIMULATIONS

In the case of the transition probability-based method, the dimension of the simulation plays a secondary role. Multi-dimensional Markov chain models are constructed assuming that spatial variability in any direction can be characterized with one-dimensional Markov chains [Lin and Harbaugh, 1984, Politis, 1994, Carle and Fogg, 1997]. This means that two perpendicular cross-sections enable the calculation of Markov chains in all three principal directions and 3D models can be built accordingly.

The way to upscale simulations for multiple-point algorithms is more complex because the search template is directly derived from the training image and the spatial correlation is not parameterized in the classical manner. Essentially, the training image must have the same dimension as the aimed simulation domain. Three dimensional training images, particularly at the scale of sand lenses, are difficult or impossible to record (Chapter 3). To simulate sand lenses in three dimensions, a methodological detour is required to account for the observed structure and anisotropy on perpendicular cross-sections.

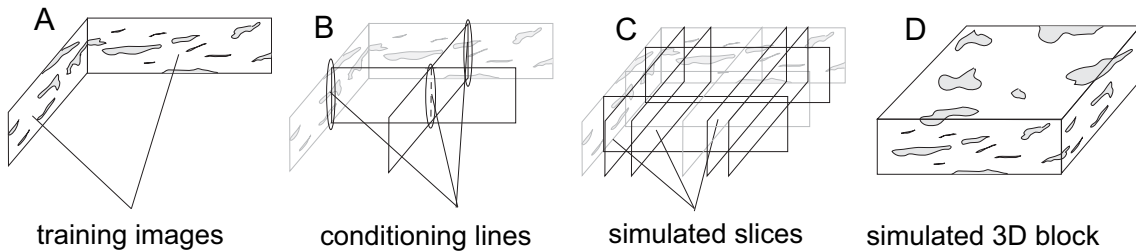


Figure 4.4: Illustration of 3D simulation path for multiple-point simulation. The 3D domain was continuously filled simulating 2D slices and condition them to the existing dataset. The outer boundaries of the domain are mapped cross-sections.

The simulation procedure starts with scanning one TI in each horizontal direction (Fig. 4.4) and defining a block fenced by mapped till sections. Subsequently, the interior is modeled with two-dimensional slices, each conditioned to the training images and to each other. This procedure is repeated until the entire domain is filled and a fully-conditioned three-dimensional block was simulated (Fig. 4.4). The methodology was described and developed further in Comunian et al. [2011a] and applied, for example, to model 3D pore space in Hajizadeh et al. [2011].

4.2.3 EVALUATION OF REALIZATIONS

The quality of realization ensembles can be evaluated by different means depending on the objectives and the simulation methods. Variogram- or covariance based methods make use of correlation measures to compare realizations. Visual inspection is particularly useful if geological conceptualizations of facies architecture are known [dell’Arciprete et al., 2011]. It is also useful to examine the effect of conditioning data on identical simulations (Fig. 4.5). If specific shapes or geobodies are simulated a statistical analysis of geometry can be beneficial. In Kessler et al. [III.] such analyses were performed trying to reproduce the histograms of size, length, thickness and anisotropy of sand lenses. A similar approach comparing the histograms of clay content levels is reported in He et al. [2009].

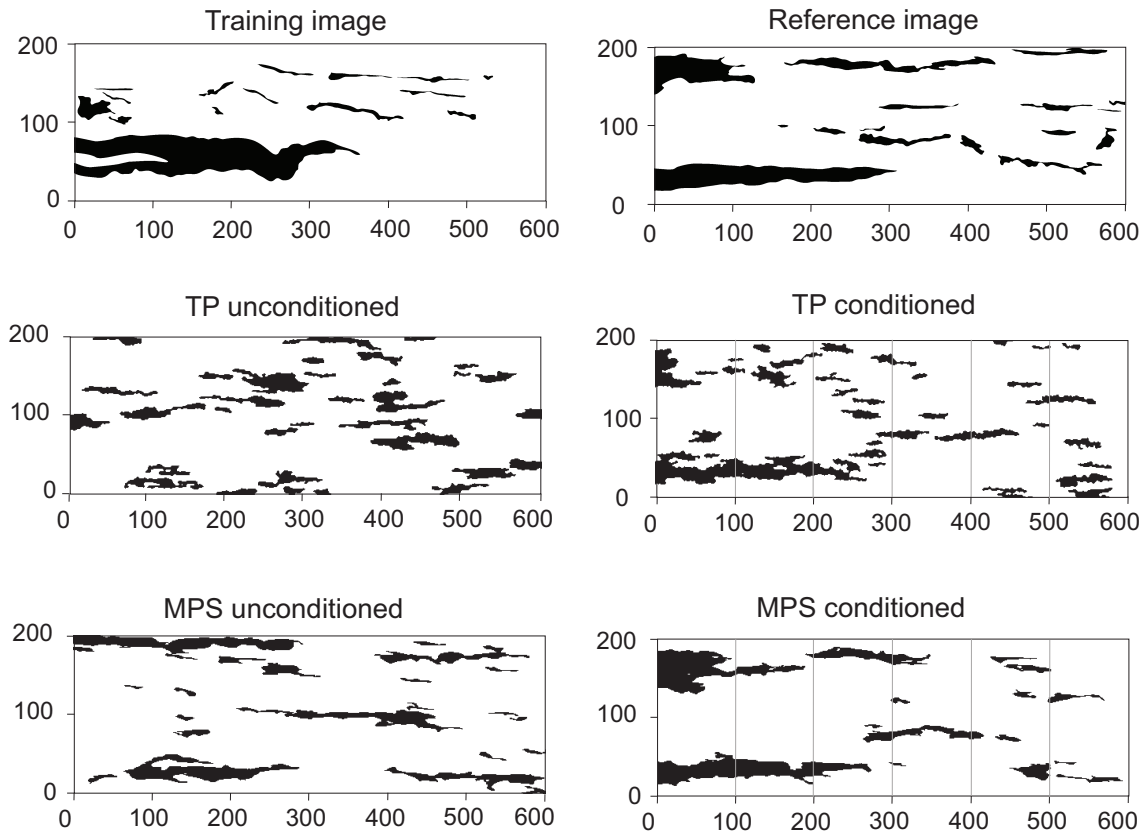


Figure 4.5: Training images and simulations of sand lenses. The upper two pictures show two till sections with sand lenses. The training image is parameterized to simulate the reference image. The simulations are performed with transition-probability-based (TP) and multiple-point statistics (MPS). The grey lines in the right image indicate columns of conditioning data, mimicking borehole logs.

Regarding the hydraulic impact of sand lenses in tills, the connectivity of features in space is of primary interest [Trinchero et al., 2008]. The measure is considered a major criterion evaluating the effect of conductive hydrofacies and was discussed in numerous geostatistical applications [Proce et al., 2004, Lee et al., 2007, Klise et al., 2009, Vassena et al., 2010, Bianchi et al., 2011, Cabello et al., 2011, Comunian et al., 2011a, Renard et al., 2011]. The relevance of connectivity measurements is demonstrated comparing multi-dimensional realizations. In two dimensions for instance, sand lenses show limited connectivity near the correlation lengths, but there are indications for connected channel networks throughout the model domain in three dimensions [Kessler et al., III.].

4.3 FINDINGS FOR SIMULATION OF SAND LENSES

Multiple-point statistics evidence enhanced performance simulating the small geometries and irregular distribution of sand lenses. The variability in size of geobodies and the strong anisotropy is better reproduced compared to two-point methods. A strict parameterization of mean lengths and proportions (TP) is rather hindering realistic simulations of individual geobodies. On the other hand, conditioning data along vertical data columns improves the visual reproduction of reference images and allows to account for increased degree of non-stationary. Three-dimensional MPS simulations require sequential simulation algorithms but are necessary to realistically evaluate the connectivity. The frequency and horizontal configuration of sand lenses indicate connectivity in three dimensions despite the small facies proportions of 10 to 20%.

5 SOLUTE TRANSPORT MODELING

Flow and solute transport models are required to perform risk assessment for contaminated sites and eventually to design effective remediation technologies [Prommer et al., 2000, Trinchero et al., 2008, Trolborg et al., 2008, Chambon et al., 2011]. The incentives of such models are the determination of plume growth and more generally the spreading of contaminants in the subsurface. Regarding remediation, transport modeling in combination with field characterizations is the crucial step to delineate the source zone and the plume extent and to locate the screen depth of monitoring or injection wells. A second aspect transport models inform about relates to the identification of relevant time scales. Remediation activities need to stay in place until the majority of contaminants are removed or degraded. Depending on the method this timeframe is determined by the combined effect of mass transfer, transport and fate of contaminants in the subsurface [Lemming et al., 2010, Manoli et al., 2012].

In relation to the study of heterogeneity, hydraulic flow and transport models serve an additional purpose. The connectivity of permeable features observed on outcrops or simulated with geostatistical methods needs to be verified with respect to the flow response. A straight-forward method is the computation of the equivalent permeability tensors [Renard and De Marsily, 1997, Renard et al., 2000]. The equivalent permeability of heterogeneous media can be remarkably increased, especially if the differences between characteristic hydraulic conductivities of hydrofacies are significant.

The connectivity and equivalent permeability indicate the relevance of conductive features for transport processes, but are yet insufficient to quantify the effect. Particle tracing and computation of breakthrough curves of contaminants provide discrete numbers for distances and time scales. Particle traces or streamlines further visualize the connected pathways through conductive hydrofacies. Examples of particle tracing in heterogeneous porous media are reported for two-dimensional cases in Klise et al. [2009] and Kessler et al. [IV.] and for three dimensions, for example, in Bianchi et al. [2011].

5.1 HYDRAULIC FRAMEWORK IN CLAYEY TILLS

Transport is controlled by the hydraulic conductivity field and the porosity of the porous media. The hydraulic properties are dependent on the geology, sediment composition and heterogeneity features. In clayey till, the matrix has a high density and very low permeability and transport is thus diffusion limited [Parker et al., 1997, Christiansen et al., 2010, Manoli et al., 2012]. Sand lenses create preferential flow paths and in this manner enhance the particle transport within the till. The difference of characteristic hydraulic conductivities can reach 4-6 orders of magnitude between the clayey matrix and the conductive sand lenses. Some representative values of hydraulic conductivity from field investigations in Danish clayey tills are shown in Fig. 5.1 and in Fredericia [1990] and Harrar et al. [2007]. Besides sand lenses, fractures occur in the upper soil horizons and create macro pores promoting advective transport in downward direction [Harrison et al., 1992, Harrar et al., 2007]. Subvertical fractures and horizontally oriented sand lenses are suspected to create a unique system of connected transport paths potentially diverting contaminants both, into deeper aquifers and in horizontal direction (Fig. 5.2).

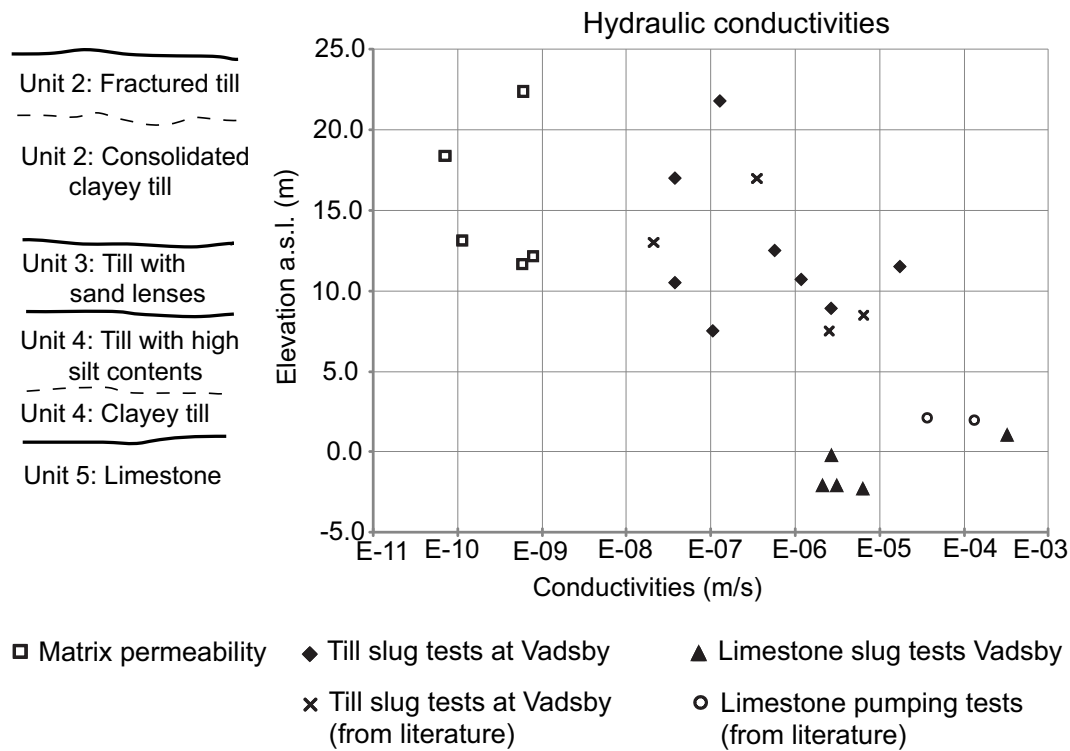


Figure 5.1: Hydraulic conductivities in clayey till. The measurements are derived from hydraulic testing at the Vadsby contaminated site. The geological stratigraphy is resolved at the left side of the picture. The geological setting corresponds to the conceptual model shown in Fig. 5.2.

5.2 INCLUSION OF HETEROGENEITY

5.2.1 IMPLEMENTATION

Advanced transport models are challenged with the degree of geological heterogeneity included. In clayey tills these are in particular fractures and sand lenses. Transport in fractured tills was modeled in a large number of studies (e.g. [Jørgensen et al., 1998, Sidle et al., 1998, Jørgensen et al., 2002, Gerke and Köhne, 2004, Jørgensen et al., 2004a, Rosenbom et al., 2009, Chambon et al., 2010]). Two concepts established themselves, 1. to treat fractured media as an equivalent porous medium (EPM), and 2. to consider two separate domains with mobile-immobile, double-porosity or double-permeability models [Berkowitz, 2002]. Models for complex transport processes were demonstrated in Sudicky and McLaren [1992], Therrien and Sudicky [1996], Graf and Therrien [2005] and Chambon et al. [2010] using discrete fracture networks.

Sand lens heterogeneity can be accounted for in transport models as separate hydrofacies. The hydraulic parameter or conductivity field (K field) is linked to the geological facies distribution as explained in Section 4. The main limitation of this approach is the lack of data. There are different approaches to account for spatially dependent K fields to overcome the data constraints. These can be ordered in terms of the amount of geological knowledge required.

1. Average K field using an equivalent porous medium
2. Random K field defining mean and variance
3. Geological facies model with characteristic K values using unconditional simulation techniques
4. Geological facies model with richer or lesser conditioning datasets

The average K field is the simplest approach averaging the hydraulic conductivity over the entire modeling domain assuming an equivalent porous medium. Bulk hydraulic conductivities are derived from hydraulic testing and yield a mean value that is usually higher than the one of the matrix itself. A more sophisticated representation is gained using random field generators. Statistical moments such as the mean and the variances of the hydraulic conductivity can be defined and even anisotropy factors are possible to implement. This method accounts for basic

geological structure, yet cannot be conditioned to field data. Stochastic simulation techniques are capable of incorporating highest degree of geological structure learning from incomplete or even external datasets. For detailed discussion of methods refer to Chapter 4. Simulations have the advantage to allocate specific K values for different hydrofacies and to allow conditioning with field data. Conditioning greatly improves the representativeness of heterogeneity models. A comparison of the four approaches to include heterogeneity into transport models is presented for sand lenses in clayey tills in Kessler et al. [IV.].

5.2.2 NUMERICAL CONSTRAINTS

In case of stochastic simulation, the heterogeneity models need to capture the geological structure which often occurs at small spatial scales. Sand lenses require a resolution of few cm to represent the complex geometries [Kessler et al., III.]. In order to avoid loss of important structure of the simulated features, the discretization of transport modeling domains must be chosen at the same or similar resolution. Modeling transport at site or even aquifer scale with high-resolution heterogeneity models entails major computing limitations because it leads exceeding numbers of model nodes.

For transport modeling of contaminated sites (point source), the way forward is to refine the discretization beneath the source and to include heterogeneity only in the relevant areas of the domain. This means to restrict heterogeneity models to the geological layers of interest and with a minimal horizontal extent in down-gradient direction. In Fig. 5.2 this idea is conceptualized for a till setting with a layer of horizontally oriented sand lenses in a specific till horizon. A simulated block of sand lenses was inserted into the model domain to evaluate the effect on the transport within the sand lenses. In Kessler et al. [IV.] this approach was tested for a 2D scenario of the same geological setting.

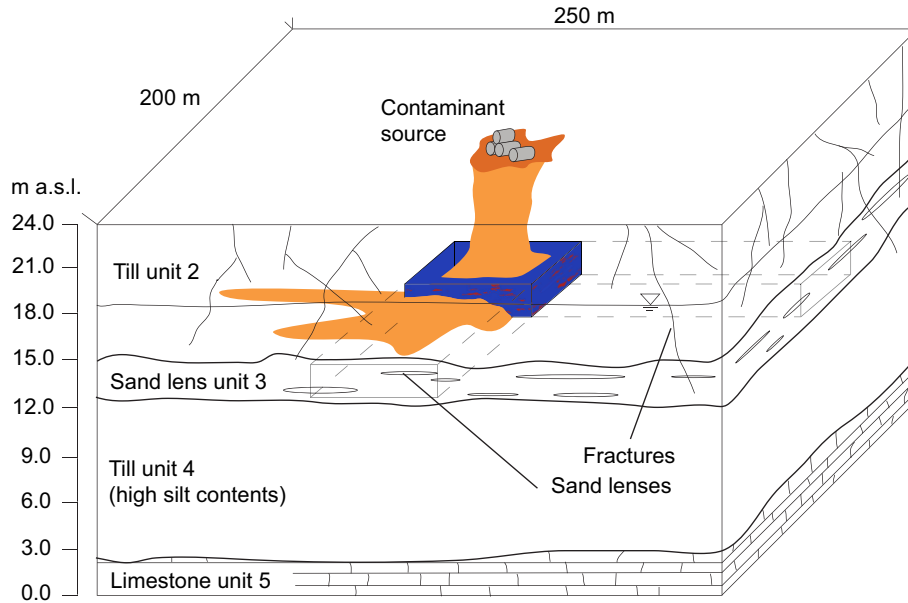


Figure 5.2: Conceptual model of solute transport in clayey till. The blue box represents a heterogeneity model of sand lenses at high resolution. It is implemented at a much smaller scale and located below the contaminant spill. The orange contamination spreads in horizontal directions once reaching the sand lenses in the blue box.

A second numerical problem arises if the characteristic hydraulic conductivities of neighboring hydrofacies differ by several orders of magnitude. Sharp transitions lead to discontinuities near the boundaries and hamper error-free transport simulations. This requires sophisticated meshing near the hydrofacies transitions further increasing the number of nodes.

5.3 CONTAMINANT TRANSPORT IN SAND LENSES

5.3.1 MODEL SCENARIO

In the described till settings, contaminants were observed to migrate preferentially into the subsurface at numerous sites [Harrar et al., 2007, Jørgensen et al., 2002, 2004b]. In Kessler et al. [IV.] a two-dimensional transport model for a synthetic case oriented at a real contaminated site was presented. The aim was to verify the hypothesized transport pattern of contaminants within sand lenses and to visualize the movement and spreading of particles. The example emphasizes on the relevant till layer interspersed with abundant sand lenses that are represented with a MPS simulation Fig. 5.2.

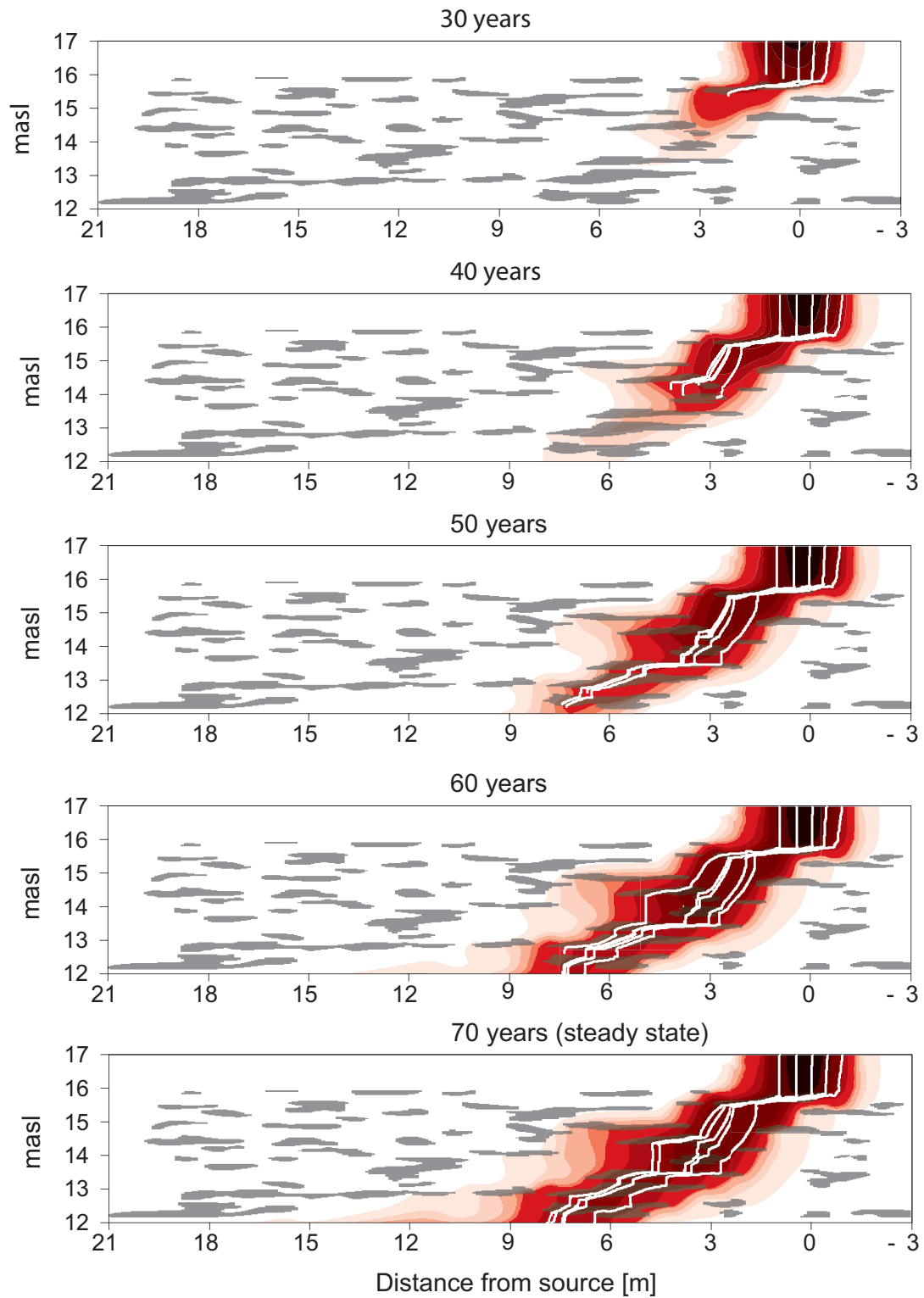


Figure 5.3: Solute transport models for clayey till in two dimensions. The representation of sand lenses was simulated with multiple-point statistics. The series of graphs illustrate the migration of contamination through a till unit interspersed with sand lenses. Steady state is reached after 70 year.

5.3.2 MODEL OUTCOMES

The time series over 50 years shows the plume growth until steady state is reached. The important observation is the specific transport paths of the particles. Instead of trickling through the medium the particles migrate stepwise downwards with a vertical component in the clay and a rather horizontal component as soon as they enter a sand lens. This means that sand lenses do facilitate horizontal transport. Further, if networks of connected lenses exist, unexpectedly large spreading and distribution of contamination is possible, despite the low equivalent permeability of clayey tills.

5.3.3 CONCLUDING REMARKS

Sand lens heterogeneity does facilitate contaminant transport in horizontal direction. The order of magnitude and scale depend on the way sand lenses or geological structure are represented. In general, the more geological data are included the more variable is the modeled contaminant transport. The MPS realizations of sand lens heterogeneity indicate the most significant horizontal spreading of contaminants because the horizontal extent of single geobodies is largest. Besides, the horizontal transport component depends on the connectivity and configuration of conductive pathways and as a result, the location of individual sand lenses relative to the source is a decisive factor. Regarding the enhanced connectivity of sand lenses in three dimensions, transport models in till settings are highly relevant to be performed in 3D.

6 CONCLUSIONS AND PERSPECTIVES

Sand lens investigations in glacial diamictons comprise several aspects starting from a geometrical characterization of single lenses to the analysis of spatial variability and the assessment of connected channel networks within the surrounding till. The presented study directed attention to each of these aspects performing field investigations and modeling exercises to describe, simulate and interpret sand lenses in a broad hydrogeological context. The key outcomes are listed below.

- The introduced methodology to characterize sand lenses includes a set of geometric parameters to capture the structure of individual lenses. The parameters length, thickness, anisotropy and orientation are sufficient to prescribe the shape and geometry and require only simple measuring tools on till outcrops.
- Sand lenses occur in all till types found in glacial landscapes, but strongly differ in their characteristics. They depict hereby the predominant deposition regimes and glaciotectonic deformation processes, and are as such a useful indicator for the identification of till types.
- Sand lenses were classified according to their geometry, genesis, grain composition and degree of deformation. The developed scheme includes sand layers, sand sheets, sand bodies, sand pockets and sand stringers, each representing characteristic lengths and properties. Most frequent are elongated and anisotropic sand pockets.
- Variogram models of till cross-sections reveal strong non-stationary patterns for sand lenses. Besides spatial trends in vertical direction, varying size of adjacent features, strong geometric anisotropy, and periodicity due to short spacing need to be considered.
- Multiple-point algorithms have remarkable advantages simulating sand lenses compared to transition probability-based geostatistics. Anisotropic and above-average features beyond the correlation length are better reproduced and closer to the observations. Spatial trends are difficult to implement with either algorithms, if based on only one cross-section or training image.
- In two dimensions the connectivity of sand lenses approximates the maximum length of single features, but no connected channel network is evident. Realizations in three dimensions, however, indicate multi-directional connectivity despite rather low proportions of 10-20% of sand facies.

- Sand lenses have commonly three orders higher hydraulic conductivity compared to the till matrix. Contaminant transport is thus controlled by preferential flow inside sand lenses. Multiple-point simulations of heterogeneity suggest the longest horizontal spread and the largest plume extent. Average or random K fields underestimate the horizontal transport because the no highly conductive features in horizontal direction are present.

The study reported in this PhD addressed several research problems and identified a number of open questions that may be of interest for further research efforts.

The classification scheme for sand lenses is mainly based on observations made at one Danish till site. Regarding the large variability of glacial processes, additional observations from different settings are required to affirm and/or extend the suggested classes. The underlying characterization is based on geometric parameters but does not inform in detail about the hydraulic properties of sand lenses. Subsequent investigations should be directed towards a hydraulic assessment of the different classes including the variability of grain size composition, porosity and hydraulic conductivity of different types of sand lenses.

Stochastic modeling of heterogeneity needs to emphasize on incorporating even more geological structure into simulations. Multiple-point algorithms were identified as the most flexible method, yet limited in terms of accounting for non-stationarity. Especially the reproduction of the spatial trends and multiple-scale features on the same training image are of interest for complicated geologies. Recently developed concepts to incorporate non-stationarity (e.g. auxiliary variables or regionalization of training images) need to be explored for sand lenses.

Regarding the increased connectivity of sand lenses in three dimensions, it is recommended to model transport processes with three-dimensional representations of heterogeneity. The horizontal transport of contaminants is controlled by conductive flow paths and connected sand lens networks may multiply the travel distance of particles. Such simulation procedures at the suggested resolution, however, require significant computing resources. Another interesting aspect is to investigate reactive transport in heterogeneous systems, because degradation processes and rates within sand lenses may vary from the ones predominating in the surrounding clayey till matrix.

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8 PAPERS

- I. Christiansen, C.M., Damgaard, I., Broholm, M.M., Kessler, T.C., Nilsson, B., Klint, K.E.S., Bjerg, P.L. (2010). Comparison of Delivery Methods for Enhanced *In Situ* Remediation in Clay Till. *Ground Water Monitoring & Remediation*, 30 (4), 107-122.
- II. Kessler, T.C., Klint, K.E.S., Nilsson, B., Bjerg, P.L. Characterization of Sand Lenses Embedded in Tills. *Quaternary Science Reviews*, in revision.
- III. Kessler, T.C., Comunian, A., Oriani, F., Renard, P., Nilsson, B., Klint, K.E.S., Bjerg, P.L. Analyzing and Modeling Fine Scale Geological Heterogeneity — an Example of Sand Lenses in Clayey Till. Submitted manuscript.
- IV. Kessler, T.C., Chambon, J.C., Binning, P.J., Nilsson, B., Klint, K.E.S., Bjerg, P.L. (2012). Implications for Risk Assessment of Sand Lenses for Solute Transport in Heterogeneous Clayey Tills. Technical note.

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